# MODELLING AND SIMULATION OF TRANSIENT COAL COMBUSTION PROCESSES IN FIXED AND MOVING GRATES

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**Abstract**—A time dependent mathematical model and a computer program have been developed to simulate coal combustion on moving and fixed grates. The physical models for both, the combustion of a single coal particle and the combustion of continuos bed of coal, have allowed a better approach to reality. The partial differential equations of the model are solved using implicit collocation and relaxation techniques, with finite differences for time advance. The program MTCC can predict several important parameters that describe the coal combustion processes in fixed and moving grates, such as composition, heat of reaction and temperature profiles for gaseous and solid phases, in the bed and the particle's interior. In addition, the program can simulate non-isothermal particles with the exposed core and non-reactive core models. The basic structure of the model includes a system of six differential equations which represent the mass and energy balances for all phases at any point along the bed.

**Keywords:** Char, grate firing, heat transfer, mathematical model.

## INTRODUCTION

Most of the commonly used models for coal combustion are stationary, isothermal in each particle,[1,2,3] and they also emphasize more on the reaction kinetics than on the heat transfer mechanism itself. The works published so far do not cover many important aspects and phenomena of the process like the thermal effects on the interphase between the unreacted coal core and the ash layer in the particles, and this fact justifies our work. This model considers simultaneously the devolatilization, drying and combustion rates in the bed,[3,4] as well as the gas production due to chemical reactions in the gaseous phase. The whole set of balances of the model can be used to assess an optimal grate velocity in the combustion equipment in order to achieve considerable energy savings. Another important fact to consider is the particle size distribution and how it evolves with time, since the heat conduction through the bed depends strongly on the particle's diameter at each point.

## MATHEMATICAL MODEL FOR COAL COMBUSTION ON GRATE

A system of several chemical reactions for a wide set of carbonaceous material-gas reactions was taken into account in the solid phase as in gases. The mathematical model was built for both, a single particle and also for a continuos system formed by the solid and gas passing through the column.

**Basic equations**

The mass and energy balance equations consider the moisture, volatil material, oxygen and heat exchange inside a single coal and also, between the bed and the gases passing through it. It also expresses that the heat released during the reaction is dissipated by convection to the gas and by conduction to the particles around. The mass balance equations for the solid and gases are

$$dm_i = R_{\alpha,i}\frac{dA_L}{d\xi}d\xi \tag{1}$$

$$\frac{dF_i}{d\xi} = R_{\alpha,i}\frac{dA_L}{d\xi} + R_{\alpha,i}\frac{dVg}{d\xi} \tag{2}$$

respectively. Concerning the energy balance, the equations are,

$$F_g C_{pg} \frac{\partial \theta_g}{\partial \xi} = h\left(\theta_c - \theta_s\right)\frac{dA_p}{d\xi} + \sum_j R_{gas,j}\frac{\Delta H_j}{\left(T_{ref} - T_{gs}\right)}\frac{dV_g}{d\xi} \tag{3}$$

$$-\frac{\partial^2 \theta_g}{\partial \xi^2} - \frac{hZ_c\left(\theta_c - \theta_s\right)}{\lambda_c(1-\varepsilon)A}\frac{dA_p}{d\xi} + \sum_i R_{sol,i}\frac{Z_c \Delta H_i}{\left(T_{ref} - T_{gs}\right)\lambda_c(1-\varepsilon)A}\frac{dA_p}{d\xi} - \frac{\partial \theta_s}{\partial r_c} = 0 \tag{4}$$

Additionally, along the bed the conservation equations for every particle must be solved. The energy equation for $r < r_N$ is stated as:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \theta_r}{\partial r}\right) + \frac{\sum \Delta H_i R_{sol,i}}{\lambda_r\left(T_{ref} - T_{gs}\right)r_N} = \frac{\rho_r C_{pr}}{\lambda_r}\frac{\partial \theta_r}{\partial t} \tag{5}$$

But for the case $r_N \leq r \leq r_p$ we must not consider the generation term. Finally, the mass equation within the particles is written as,

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \rho_v}{\partial \rho}\right) + \frac{R_{sol,i}}{r_N D_{ef}} = 0 \tag{6}$$

**Boundary conditions**

The gas temperature at the reactor's entrance does not vary with time and the coal temperature at the same point will be constant as well, when the coal feeding is continuous. Coal temperature at the reactor entrance will depend on time when it is a batch process. On the other hand coal temperature on the top of the bed is subjected to radiation conditions and the length of the coal bed depends upon the coal consumption rate. The boundary conditions for chemical species are known at the entrance of the reactor for air and they are also initial conditions for Carbon.

The computer program MTCC was developed for modeling both, reactive and non-reactive core particles. For the non-reactive model we have to apply a continuity condition between the core and the ash layer, however this is unnecessary for the exposed-core model. In addition, for both models we need to apply symmetry at the center and a Dirichlet condition on the surface to assess convection effects. Most physical properties were calculated using the Chilton-Colburn analogy,[5] while some expressions as the diffusion coefficient and specific area can be found in references 3,6,7,8.

**Reaction kinetics**

The model includes the set of chemical reactions from the references 8 and 9. Models for gas-solid reactions: These models deal with drying and devolatilization and in this work we modified and used them in transient stages of combustion including in the analysis the growth rate of the ash layers.

Drying and devolatilization processes: The non-reactive core model is analysed. For the devolatilization case it was necessary to perform a mass balance with the different gases being generated in this stage and the remaining mass in the coal bed.

Mass and heat transfer: There are many useful analogies that considers the effects of solid-fluid heat and mass transfer coeffients in the process, as presented by Bird, Stewart, Lightfoot, and others.[10,11,12] In the simulation program all these coefficients depend on the temperature, composition and flows along the solid bed, and therefore they are constantly changing with position and time.

## DESCRIPTION OF THE SIMULATION PROGRAM

The basic necessary input data for the program are: Complete physical and chemical characterization of the fed coal, composition and temperature of the primary air at the entrance, basic geometry and dimensions, i.e. reactor diameter, bed length, flow parameters as bed porosity, pressure head and other physical properties.

The numerical method was a combination of collocation[13] and relaxation. In the collocation method, each variable is written as linear combination of a set of non-linear interpolating functions, which depend on the spatial coordinates. For example, in the present work the equations have the general form,

$$\frac{\partial f}{\partial t} = A\frac{\partial^2 f}{\partial z^2} + B\frac{\partial f}{\partial z} + C \tag{7}$$

where $A$,$B$, and $C$ are functions of temperature , composition and time and with the variable $f$ assumed to be,

$$f_j = \sum_{i=1}^{N} a_i F_{ij} \tag{8}$$

where $f_j$ states for the variable $f$ at node j, and N is the number of collocation points. The method has the advantages that the collocation points can be generated anywhere in the integration domain and a symmetric and well posed coefficient matrix is generated and easily inverted. The collocation method uses radial local functions between the collocation point and the other point in the domain.

Equation (8) is substituted into differential equation (7), and in this manner a set of N equations with N unknowns is obtained, where N is the number of nodes and the unknowns are the coefficients of the linear combination (8). On the other hand, the time term is discretized in finite differences using upwinding schemes.

The initial step is to transform the differential equations into a equivalent set of differential equations of first order by an adequate change of variable[14,15]. Thus the aspect of the final equations to be solved is,

$$\frac{\partial Y}{\partial t} = \{a\} Y = G(Y) \tag{9}$$

where $\{a\}$ is the coefficient matrix and $Y_i$ is the vector of temperatures and heat fluxes at node i. Next, the first order derivatives are discretized in finite differences, and the resulting truncation error expands in Taylor series,

$$E_k(Y + \Delta Y) = E_k(Y) + \sum_{i=1}^{N} \frac{\partial E_k}{\partial Y_{i,k-1}} \Delta Y_{i,k-1} + \sum_{i=1}^{N} \frac{\partial E_k}{\partial Y_{i,k}} \Delta Y_{i,k} \tag{10}$$

$E_k$ is the truncation error at the same node. By means of an iterative algorithm, the error is minimised based not only on the values of the position along the bed but also on the values of temperatures $T_g$ and $T_s$ and concentrations at each node.

## RESULTS

In transient state, temperature rises due to energy transfer within the solid and gases plus the thermal energy generation by chemical reactions as shown in figures 1,2 and 3.

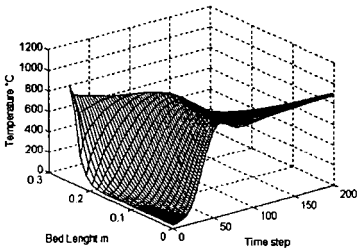


Figure 1. Temperature of the solid as function of time and position. Time step = 200 s

On the other hand, the composition of the gaseous mixture changes strongly with time. The oxygen $O_2$ decreases for the oxidation of Carbon to produce $CO_2$ and then it increases again because the air flow is constant while the Coal is consumed (figures 4,5).

In figure 6 the amount of water in combustion gases is depicted. Water and Oxygen play an important role influencing how much CO (figure 7) is obtained during combustion, however as a general rule the evolution of CO and $CO_2$ are alike.

Finally, during the entire process growing amounts of $NO_x$ and $SO_2$ coming form the Coal were observed (Figures 8-9).

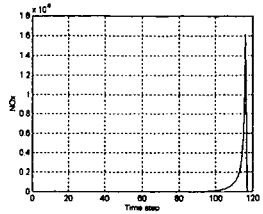


Figure 2. Fraction of NOx in gases growing with temperature and time.

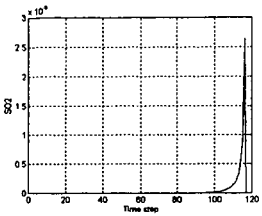


Figure 3. Fraction of SO2 in gases.

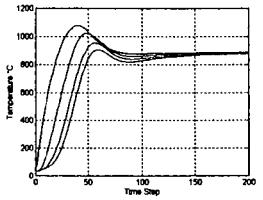


Figure 4. Coal temperature as function of time at different posotions along the bed. Time step =200 s

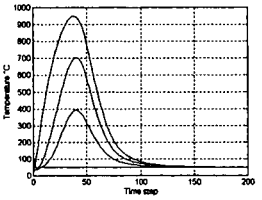


Figure 5. Gas temperature as fuctions of time at different positions along the bed. Time step= 200 s

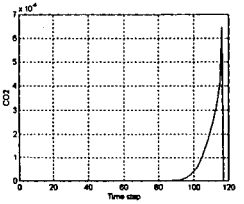


Figure 6. Carbon dioxide fraction in gases at the entrance of the reactor

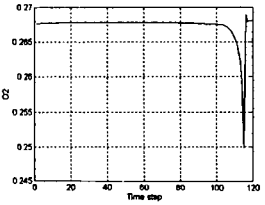


Figure 7. Oxygen fraction in gases at the entrance of the reactor

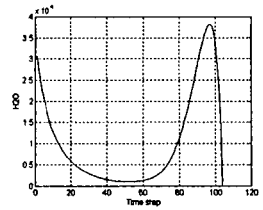


Figure 8. Fraction of water during combustion as function od time. Time Step =200 s

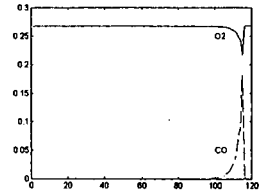


Figure 9. Relation between Oxygen and CO as time progresses. Time step=200 s

## CONCLUSIONS

The computational model will allow us to predict the combustion stages and eventually the production of unburned material due to oxygen deficiency. The cases analysed here correspond to enough oxygen such that there is not unburned material

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## NOMENCLATURE

$[O_2]^*_{S,G}$ = Oxygen concentration in gas stream
$\Delta H_{rxn}$ = Carbon combustion enthalpy
$[O_2]$ = Oxygen concentration
$[O_2]_e$ = Oxygen concentration inside coal
$a$ = Coal bed specific area
$A_p$ = Particle area
$C_{pg}$ = Gas specific heat
$D_{O2}$ = Oxygen diffusion coefficient
f = Remaining coal fraction in the bed
$F_g$ = Gas flow
$G_g$ = Air flow mass
h = Convective heat transfer coefficient
$K_{ef}$ = Coal thermal conductivity
$K_m$ = Mass transfer coefficient
Kr = Reaction rate
$M_c$ = Mass per unit volume of the coal particle
$M_{mc}$ = Carbon molecular weight
$M_o$ = Initial mass per unit volume of the coal particle
$M_{O2}$ = Oxygen molecular weight.
$N_p$ = Number of particles per unit volume
r = Radius of the non reactive particle nucleus
$R_{gg}$ = Gas-gas reaction rate
$R_{sg}$ = Solid-gas reaction rate
$T_c$ = Solid temperature
$T_{co}$ = Initial solid temperature
$T_g$ = Gas temperature
$T_{go}$ = Gas temperature at the entrance
$V_g$ = Gas volume
Z = Axial bed distance
$Z_o$ = Initial bed height

*Greek letters*

$\rho_g$ = Gas density
$\varepsilon_p$ = Coal porosity
$\alpha$ = Thermal diffusivity
$\xi$ = Dimensionless axial coordinate
$\rho$ = Dimensionless radius
$\theta_c$ = Dimensionless coal temperature
$\lambda_{CZ}$ = Ash thermal conductivity
$\theta_g$ = Dimensionless gas temperature